An Equation-Free Approach to Nonlinear Control: Coarse Feedback Linearization With Pole-Placement

Constantinos I. Siettos [1]

Department of Chemical Engineering, Princeton University, Princeton, NJ 08544
Electronic mail address: ksiet@mail.ntua.gr

Ioannis G. Kevrekidis[2]

Department of Chemical Engineering, Department of Mathematics and Program in Computational and Applied Mathematics, Princeton University, Princeton, NJ 08544
Electronic mail address: yannis@princeton.edu

Nikolaos Kazantzis

Department of Chemical Engineering, Worcester Polytechnic Institute, Worcester, MA 01609-2280, Electronic mail address: nikolas@wpi.edu

Abstract

We present an application of equation-free computation to the coarse-grained feedback linearization problem of nonlinear systems described by microscopic/stochastic simulators. Feedback linearization with pole placement requires the solution of a functional equation involving the macroscopic (coarse-grained) system model. In the absence of such a closed-form model, short, appropriately initialized bursts of microscopic simulation are designed and performed, and their results used to estimate on demand the quantities required for the numerical solution of the (explicitly unavailable) functional equation. Our illustrative example is a kinetic Monte Carlo realization of a simplified heterogeneous catalytic reaction scheme.

[1] *Currently: School of Applied Mathematics and Physics, National Technical University of Athens, Zografou Campus, Athens, GR 157 80, Greece*
[2] Author to whom correspondence should be directed

1 Introduction

A fundamental prerequisite for the design of control systems is the availability of reasonably accurate closed form dynamical models. Typically, such models arise in the form of evolution equations (ordinary differential, differential algebraic, partial differential, possibly integrodifferential equations). Such equations are typically derived from conservation laws (e.g. mass, momentum and energy balances) closed through constitutive equations (e.g. Newtonian stresses in fluid flow, or mass-action kinetics expressions for chemical reactions); system identification may also play a role in obtaining and/or closing such macroscopic models. Many real-world problems of current engineering interest are characterized -due to their stochastic/microscopic nature, and nonlinear complexity- by the lack of such good explicit, coarse-grained macroscopic evolution equations. Instead, the underlying physics description may be available at a much *finer*, more detailed level: the evolution rules may be given in the form of molecular dynamics, kinetic Monte Carlo, Markov-chain or hybrid schemes. When this is the case, conventional continuum algorithms cannot be used directly for systems level analysis and controller design. Bridging systematically the enormous gap between microscopic space and time scales of a complex physical/material system description and the macroscopic ones at which we want to design and control its behavior is a grand challenge for modeling and computation. Over the past few years we have demonstrated that an equation-free approach (based on coarse timesteppers) [Theodoropoulos et al., 2002; Makeev et al.,2002; Kevrekidis et al., 2003; Siettos et al., 2003b; Kevrekidis et al., 2004], can establish a link between traditional continuum numerical analysis and microscopic/ stochastic simulation. This is a mathematics-assisted computational methodology, inspired from continuum numerical analysis, system identification and large scale iterative linear algebra, which enables microscopic-level codes to perform system-level analysis directly, without the need to pass through an intermediate, coarse-grained, macroscopic-level, "conventional" description of the system dynamics. The backbone of the method is the *on-demand* identification of the quantities required for continuum numerics (coarse residuals, the action of coarse slow Jacobians, eigenvalues, Hessians, etc). These are obtained by repeated, appropriately initialized calls to an existing *fine scale* time-stepping routine, which is treated as an input-output black box. The key assumption is that deterministic, macroscopic, coarse models exist and close for the expected behavior of a few macroscopic system observables, yet they are unavailable in closed form. These observables (coarse-grained variables) are typically a few low moments of microscopically evolving distributions (e.g. surface coverages, the zeroth moments of species distributions on a lattice

model of a surface reaction).

The present work aims at developing a systematic approach to the feedback regulator synthesis problem, where both the closed-loop dynamics linearization and pole-placement objectives are simultaneously attained by using the equation-free timestepper methodology. The feedback linearization and the pole-placement objectives for the unavailable coarse-grained dynamics are met in a *single-step*, circumventing the lack of an explicit dynamic process model. The proposed approach is illustrated through the use of a coarse time-stepper based on a kinetic Monte Carlo realization of a simplified surface reaction scheme for the dynamics of NO oxidation by H_2 on Pt and Rh surfaces. The present paper is organized as follows: In section 2 we briefly discuss the traditional nonlinear control methodologies that rely on the notion of feedback linearization along with the associated restrictions encountered at the implementation stage. In section 3 we succinctly review a recently proposed approach that allows the attainment of both the feedback linearization and pole placement objectives in a single step, effectively overcoming the restrictive conditions associated with the classical exact feedback linearization approach. In section 4 the interplay of the proposed nonlinear control procedure with coarse timesteppers is outlined, and the natural integration of the respective frameworks illustrated. Section 5 presents the simulation results using the proposed methodology on an illustrative kinetic Monte Carlo model, followed by some concluding remarks in section 6.

2 Fundamentals of feedback linearization of nonlinear systems

In order to meet a set of performance specifications or design objectives, process control introduces feedback to appropriately modify the dynamics of a system. Placing the closed-loop poles at desirable locations in the complex plane, and thus shaping the closed loop system dynamics and time constants, is a popular controller synthesis method for linear systems, in part, due to its intuitive appeal [Chen, 1984]. Typically one requires fast decay of the closed loop variables to their nominal steady state values; yet the design should not lead to high feedback gains due to possible saturation problems. Fine-tuning of the closed-loop eigenvalues is performed in practice through a combination of optimization techniques, heuristic rules and trial-and-error approaches [Chen, 1984]. Traditional pole-placement state feedback control laws for nonlinear systems are based on local linearization around a reference steady state, and the subsequent use of linear design methods. The results are, of course, only locally valid, and may lead to unacceptable performance, even in the presence of only mild nonlinearities. Nonlinear feedback control laws thus need to be

derived, capable of directly coping with the system nonlinearities. A pole-placing feedback regulator should be capable of bringing the system/process state back to the design steady state in a fast and smooth manner in the presence of disturbances; if the design steady state is unstable, the primary control objective is its stabilization. In the pertinent body of literature two main model-based pole-placing controller synthesis methods emerge, both based on geometric control theory. The first one is exact input/output (I/O) feedback linearization, where the introduction of nonlinear state feedback induces linear I/O behavior of the system of interest, forcing the system's output to follow a prespecified linear and stable trajectory. This approach directly generalizes the linear result of placing the closed-loop poles at the system's zeros and at a set of prespecified values, and is restricted within the class of minimum-phase systems [Isidori, 1999]. Regulation and/or stabilization of a system/process, however, is understood in terms of forcing the system's state to return to the design steady state (if driven away from it in the presence of disturbances). Furthermore, process output tracking problems for step changes in the output set-point values, can be easily reformulated as regulation problems relative to the equilibrium point that corresponds to the final set-point value. The second approach is geometric exact feedback linearization, traditionally implemented in a two-step design procedure [Isidori, 1999]: A simultaneous implementation of a nonlinear coordinate transformation and a state feedback control law in the first step transforms the original nonlinear system to a linear and controllable one. Well-established linear pole-placement techniques for the transformed linear system can be used in the second step. However, the aforementioned classical geometric exact feedback linearization approach relies on a set of very restrictive conditions, that can hardly be met by any physical system.

In this work a systematic approach to feedback regulator synthesis is proposed for the coarse-grained dynamic behavior of systems described by atomistic/stochastic ("fine scale") simulators. The closed-loop dynamics linearization and the pole-placement objectives are simultaneously attained using the equation-free timestepper-based methodology. Note that our primary control objective is to assign the closed-loop eigenvalues rather than shaping the entire I/O behavior of the system under consideration. Furthermore, applying the methodology introduced in [Kazantzis, 2001], we investigate the possibility of circumventing the set of restrictive conditions associated with the two-step classical exact feedback linearization approach, by meeting the feedback linearization and the pole-placement objectives in a **single-step**, and without being limited by the availability of an explicit dynamic process model.

3 Mathematical Preliminaries - Problem Formulation

In the context of the present study, the system dynamics are described by a nonlinear discrete-time macroscopic ("coarse") model of the form:

$$x(k+1) = \Phi(x(k), u(k)). \tag{1}$$

Here $k \in N^+ = \{0, 1, ...\}$ is the discrete-time index, $x(k) \in R^n$ is the vector of (coarse) state variables, $u(k) \in R$ is the manipulated input variable and $\Phi(x, u)$ represents a vector function defined on $R^n \times R$. In our case this function is not known, and will be identified on the fly with the aid of the fine scale simulator. Without loss of generality, it is assumed that the origin $x^0 = 0$ is an equilibrium point (coarse steady state) of (1), that corresponds to $u^0 = 0$: $\Phi(0, 0) = 0$. If a non-zero coarse steady-state $(x^0, u^0) \neq (0, 0)$ is located, then a simple transformation: $\hat{x} = x - x^0, \hat{u} = u - u^0$ will map it to the origin in the new coordinate system. Let F be the Jacobian matrix of $\Phi(x, u)$ evaluated at $x = 0$: $F = \dfrac{\partial \Phi}{\partial x}(0, 0)$, and G the vector: $G = \dfrac{\partial \Phi}{\partial u}(0, 0)$ which is assumed to be non-zero. The following assumption is also made:

Assumption I: The $n \times n$ matrix:

$$\mathcal{C} = [\, G | FG | ... | F^{n-1} G \,] \tag{2}$$

has rank n. This implies that the coarse linearization of (1) around the origin $x = 0$ is controllable [Isidori, 1999].

It is appropriate, at this point, to briefly review and outline basic features of the classical exact feedback linearization approach in the discrete-time domain. In the first step, and under a set of rather restrictive conditions [Aranda-Bricaire et al., 1996; Califano et al., 1999; Grizzle, 1986; Jacubczyck, 1987; Lee et al., 1987; Lin and Brynes, 1995; Nam, 1989], a nonlinear coordinate transformation: $z = T(x)$ is sought along with a state feedback control law: $u = \Psi(x, v)$ (with v being an external reference input), such that the original system (1) is transformed to the following linear one:

$$z(k+1) = Az(k) + bv(k) \tag{3}$$

where (A, b) is a Brunowsky controllable pair of matrices [Chen, 1984]. In the second step, standard linear pole-placing feedback techniques are used to arbitrarily assign the poles (equivalently the time-constants) of the closed-loop system. In particular, a constant-gain vector K is calculated, such that the state feedback law: $v = -Kz$ induces the desirable closed-loop dynamics:

$$z(k+1) = \bar{A} z(k) = (A - bK) z(k) \tag{4}$$

with $\bar{A} = A - bK$ being the closed-loop system's characteristic matrix with prescribed eigenvalues.

At this point it would be appropriate to review an alternative *single-step* design method for linear systems:

$$x(k+1) = Ax(k) + bu(k), \tag{5}$$

where A, b are constant matrices with appropriate dimensions, that was first introduced by D. Luenberger (1963). This alternative approach serves as the methodological basis for the development of a nonlinear analogue introduced in [Kazantzis, 2001] and briefly outlined in the next section. According to the ideas reported in [Luenberger, 1963] a single-step simultaneous implementation of a linear coordinate transformation: $z = Tx$ coupled with a linear state feedback control law: $u = -Kz$ is sought, that induce the following closed-loop dynamics:

$$z(k+1) = \bar{A}z(k) \tag{6}$$

$\bar{A}$ is the closed-loop system's characteristic matrix that carries the prescribed set of eigenvalues due to the control law applied. This requirement can be mathematically translated into a quadratic matrix equation that the unknown transformation matrix T should satisfy:

$$TA - \bar{A}T = TbKT \tag{7}$$

If T is non-singular (invertible), one can easily show that the inverse transformation matrix $W = T^{-1}$ satisfies the following linear matrix equation:

$$AW - W\bar{A} = bK. \tag{8}$$

It is known from linear algebra that, if matrices A and $\bar{A}$ have disjoint eigenspectra, the above matrix equation (8) admits a unique solution W [Chen, 1984; Gantmacher, 1960]. Furthermore, invertibility of the solution can be ensured iff the pair of matrices (A, b) is controllable and the pair $(K, \bar{A})$ is an observable one [Chen, 1984]. As shown in [Luenberger, 1963], if T is the unique invertible solution to the matrix equation (7), then the linear state feedback control law expressed in the original variables x

$$u(k) = -KTx(k) \tag{9}$$

induces the closed-loop dynamics:

$$x(k+1) = T^{-1}\bar{A}Tx(k) \tag{10}$$

Since matrices $T^{-1}\bar{A}T$ and $\bar{A}$ are similar, it can be easily inferred that the closed-loop system has the desirable set of poles assigned by the control law (9).

3.1 Single-Step Feedback Linearization With Pole-Placement

Motivated by D. Luenberger's linear approach [Luenberger, 1963], let us now succinctly review the ideas presented in [Kazantzis, 2001] on its nonlinear generalization. One seeks to simultaneously implement a nonlinear coordinate transformation, $z = S(x)$ coupled with a nonlinear state feedback control law, $u = -cz = -cS(x)$, where c is an arbitrary constant row vector (a design parameter of the proposed method) that induce linear closed-loop z-dynamics:

$$z(k+1) = Az(k). \tag{11}$$

The poles of the closed-loop dynamics (11) are realized by the eigenvalues of the arbitrarily prescribed matrix A: the characteristic matrix of the linear closed-loop dynamics (11). Therefore, the eigenspectrum of A should be judiciously selected to favorably shape the dynamic characteristics of the controlled system's response. In the nonlinear case, these design requirements are embodied into the following system of nonlinear functional equations (NFEs) that need to be satisfied by the unknown transformation map $S(x)$:

$$\begin{aligned} S(\Phi(x, -cS(x))) &= AS(x) \\ S(0) &= 0. \end{aligned} \tag{12}$$

The accompanying initial condition $S(0) = 0$ merely reflects the fact that equilibrium properties must be preserved under the proposed coordinate transformation.

For the study of the mathematical properties of the solution of the NFEs (12) and within the class of real analytic systems, a number of assumptions are essential as shown in [Kazantzis, 2001]:

Assumption II: All the eigenvalues $k_i, (i = 1, ..., n)$ of matrix A should lie inside the unit disc on the complex plane (stability requirement imposed on the closed-loop dynamics (11)).

Assumption III: The eigenspectra $\sigma(A), \sigma(F)$ of matrices A and F respectively should be disjoint: $\sigma(A) \cap \sigma(F) = \emptyset$.

Assumption IV: The eigenvalues k_i of A should not be related to the eigenvalues $\lambda_j, (j = 1, ..., n)$ of F through any equations of the type:

$$\prod_{i=1}^{n} k_i^{m_i} = \lambda_j \tag{13}$$

$(j = 1, ..., n)$, where all the m_i's are non-negative integers that satisfy the condition:

$$\sum_{i=1}^{n} m_i > 0. \tag{14}$$

Assumption V: The pair of matrices (c, A) is chosen such that the following matrix O:

$$O = \begin{bmatrix} c \\ cA \\ . \\ . \\ cA^{n-1} \end{bmatrix} \tag{15}$$

has rank n: $\text{rank}(O) = n$ (Observability condition imposed on (c, A)).

Lemma: [Kazantzis, 2001] *For a real analytic system (1), let the above assumptions I-V hold true. Then, the system of NFEs (12) admits a unique locally analytic and invertible solution $z = S(x)$ in a neighborhood of the origin $x = 0$.*

We include here a number of remarks discussing the conditions and implications of this Lemma; a more detailed discussion can be found in [Kazantzis, 2001].

Remark 1: The "non-resonance" conditions (13) and (14) are required for the existence of a unique formal power-series solution to the system of NFEs (12). The assumption for the eigenspectrum of matrix A to lie inside the unit disc plays a key role in the uniform convergence of this formal power-series solution in the neighborhood of the origin $x = 0$ with a non-zero radius of convergence, and thus for the solution's analyticity. Finally, Assumptions I and V are necessary and sufficient conditions for local invertibility of the solution.

Remark 2: It is useful to consider the linear case: $\Phi(x, u) = Fx + Gu$ where F, G are a constant matrix and vector of appropriate dimensions respectively. In this case, the unique solution of the system of NFEs (12) is $w = \mathcal{S}x$, where $\mathcal{S}$ is the solution to the quadratic matrix equation:

$$\mathcal{S}F - A\mathcal{S} = \mathcal{S}Gc\mathcal{S}. \tag{16}$$

which coincides with (7) in D. Luenberger's analysis. Please notice, that under the assumptions stated the above matrix equation (16) admits a unique and invertible solution $\mathcal{S}$ [Chen, 1984].

Let us now consider: $z = S(x)$ to be the solution to the associated system of NFE's (12) defined in a neighborhood of $x = 0$. It has been shown in Kazantzis (2001) that the simultaneous implementation of the nonlinear coordinate transformation: $z = S(x)$ and the nonlinear state feedback control law:

$$u(k) = -cS(x(k)) \tag{17}$$

results in linear closed-loop z-dynamics:

$$z(k+1) = Az(k) \tag{18}$$

whose poles are realized by the eigenvalues of matrix A. Indeed, one can easily show that the closed-loop system dynamics expressed in the z-coordinates satisfy:

$$\begin{aligned} z(k+1) &= S(x(k+1)) = S(\Phi(x(k), -cS(x(k))) \\ &= AS(x(k)) = Az(k). \end{aligned} \tag{19}$$

Remark 3: Note that in the linear case, one calculates a feedback control law:

$$u(k) = -c\mathcal{S}x(k) \tag{20}$$

where $\mathcal{S}$ is the solution to (16), that induces the following closed-loop dynamics:

$$x(k+1) = (F - Gc\mathcal{S})x(k) \tag{21}$$

Using equation (16), the closed-loop dynamics (21) can be rewritten as follows:

$$x(k+1) = (\mathcal{S}^{-1}A\mathcal{S})x(k) = \tilde{A}x(k). \tag{22}$$

Notice that $A, \tilde{A} = \mathcal{S}^{-1}A\mathcal{S}$ are similar matrices, and therefore, the closed-loop system (22) has the desirable poles. One can consider this approach as the natural extension of D. Luenberger's linear result for pole-placement (10) to nonlinear systems.

Remark 4: The graph of the mapping $z = S(x)$ is rendered invariant for the composite system (1) and (11) under the state feedback control law: $u(k) = -cS(x(k))$ [Carr, 1981]. Furthermore, the system of NFEs (12) represent the associated invariance functional equations for the composite system (1)-(11) [Guckenheimer and Holmes, 1983], and the restriction of the composite system dynamics under the above feedback law on the invariant manifold/solution of (12) coincides with the linear closed-loop dynamics (11).

Remark 5: The primary idea of the proposed single-step design approach is to avoid the intermediate step of transforming the original system into a linear controllable one with an external reference input, which allowed us to circumvent the restrictive conditions associated with the classical exact feedback linearization method [Aranda-Bricaire, 1996; Califano, 1999; Grizzle, 1986; Jakubczyck, 1987; Lee, 1987; Lin and Byrnes, 1995; Nam, 1989]. It should be pointed out, that the design method described does not involve an external reference input, however, and therefore other control objectives such as trajectory tracking or model matching can not be met [Isidori, 1999].

In the present study the NFEs (12) will be solved using the equation-free computational framework. However, for completeness and comparative accuracy, one needs to employ a alternative solution scheme/method for the system of NFE's (12). This method involves expanding $\Phi(x, u)$ as well as the unknown solution $S(x)$ in a Taylor series and equating

the Taylor coefficients of the same order of both sides of the NFE's (12). This procedure leads to linear recursion formulas, through which one can calculate the N-th order Taylor coefficients of $S(x)$, given the Taylor coefficients of $S(x)$ up to the order $N-1$. As shown in [Kazantzis, 2001], in the derivation of the recursion formulas, it is convenient to use the following tensorial notation:

a) The entries of a constant matrix A are represented as a_i^j, where the subscript i refers to the corresponding row and the superscript j to the corresponding column of the matrix.

b) The partial derivatives of the μ-th component $\Phi_\mu(x,u)$ of the vector function $\Phi(x,u)$ with respect to the state variables x evaluated at $(x,u)=(0,0)$ are denoted as follows:

$$\begin{aligned} f_\mu^i &= \frac{\partial \Phi_\mu}{\partial x_i}(0,0) \\ f_\mu^{ij} &= \frac{\partial^2 \Phi_\mu}{\partial x_i \partial x_j}(0,0) \\ f_\mu^{ijk} &= \frac{\partial^3 \Phi_\mu}{\partial x_i \partial x_j \partial x_k}(0,0) \end{aligned} \tag{23}$$

etc., where $i,j,k,..=1,...,n$

c) The partial derivatives of the μ-th component $\Phi_\mu(x,u)$ of the vector function $\Phi(x,u)$ with respect to the input variable u evaluated at $(x,u)=(0,0)$ are denoted as follows:

$$g_\mu^i = \frac{\partial^i \Phi_\mu}{\partial u^i}(0,0) \tag{24}$$

etc.

d) The standard summation convention where repeated upper and lower tensorial indices are summed up.

Under the above notation the l-th component $S_l(x)$ of the unknown solution $S(x)$ can be expanded in a multivariate Taylor series as follows:

$$\begin{aligned} S_l(x) &= \frac{1}{1!} S_l^{i_1} x_{i_1} + \frac{1}{2!} S_l^{i_1 i_2} x_{i_1} x_{i_2} + ... + \\ &+ \frac{1}{N!} S_l^{i_1 i_2 ... i_N} x_{i_1} x_{i_2} ... x_{i_N} + ... \end{aligned} \tag{25}$$

Similarly one expands the components of the vector function $\Phi(x,u)$ in multivariate Taylor series. Substituting the Taylor expansions of $S(x)$ and $\Phi(x,u)$ into (12) and matching the Taylor coefficients of the same order, the following relation for the N-th order terms may be obtained [Kazantzis, 2001]:

$$\sum_{L=1}^{N} \sum_{\substack{0 \le m_1 \le m_2 \le ... \le m_L \\ m_1 + m_2 + ... + m_L = N}} S_l^{j_1 ... j_L} (f_{j_1}^{m_1} ... f_{j_L}^{m_L} - \pi_{j_1}^{m_1} ... \pi_{j_L}^{m_L}) = a_l^\mu S_\mu^{i_1 ... i_N} \tag{26}$$

where:

$$\pi_{jl}^{m_L} = \sum_{P=1}^{L} \sum_{\substack{0\le n_1 \le n_2 \le \ldots \le n_P \\ n_1+n_2+\ldots+n_P=m_L}} g_{jl}^{n_1} c^k S_k^{n_2\ldots n_P} \tag{27}$$

$i_1, ..., i_N = 1, ..., n$ and $l = 1, ..., n$. Notice that the second summation symbol in (26) (and similarly in (27)) suggests summing up the relevant quantities over the $\dfrac{N!}{m_1!...m_L!}$ possible combinations to assign the N indices $(i_1, ..., i_N)$ as upper indices to the L positions $\{f_{j_1}, ...f_{j_L}\}$ (and $\{\pi_{j_1}, ...\pi_{j_L}\}$), with m_1 of them being put in the first position, m_2 of them in the second position , etc. $(\sum_{i=1}^{L} m_i = N)$. Moreover, notice that equations (26,27) represent a set of linear algebraic equations in the unknown coefficients $S_\mu^{i_1,...,i_N}$ for $N \geq 2$. For $N = 1$, equations (26,27) yield the quadratic matrix equation (16) (or (7) in D. Luenberger's approach). It should be pointed out, that the above series solution method for the NFE's (12) is amenable to a computer-based implementation and can be readily carried out in an automatic fashion with the aid of a symbolic software package such as MAPLE.

4 An Equation-Free Approach to the Feedback Linearization Problem

As shown in the previous section, the system of NFEs (12) admits a unique analytic solution. However, such an analytic transformation is difficult to derive in the general case, and a numerical solution scheme becomes necessary. We will now assume that the model equations are not explicitly available, but we do have a "black box" subroutine that, given the state of the system $x_0 \in R^n, u_0 \in R$ at time $t_k = kT$ reports the result of the system after a time horizon T (i.e., will report $x(t_{k+1} = (k+1)T) \equiv \Phi_T(x_0, u_0))$. This subroutine could be a "legacy" dynamic simulator; alternatively, it can be a "coarse timestepper" involving the lift, run and restrict steps discussed briefly below and in more detail in [Makeev et al., 2002; Gear et al., 2002; Kevrekidis et al. 2003, Siettos et al., 2003b]. The coarse timestepper, which we use in the equation-free framework for coarse-grained controller design (for linear quadratic control, pole placement and feedback linearization) [Siettos et al., 2003a, Siettos, et al., 2004a, Armaou et al., 2004a, 2004b, Siettos et al., 2004b] consists of the following elements (Figure 1):

- a lifting operator μ, transforming a macroscopic initial condition (typically zeroth- or first-order moments of the microscopically evolving distributions) to one (or more) consistent microscopic realizations;
- evolution of the microscopic realizations using the microscopic simulator for an appro-

priately chosen (relatively short) macroscopic time T, (*the reporting horizon*).

- a restriction operator M, transforming the resulting microscopic distributions back to the macroscopic description (obtaining their macroscopic observables). Lifting from microscopic to the macroscopic and then restricting again should have theoretically no effect (modulo roundoff), that is, $\mu M = I$.

This coarse timestepper, appropriately initialized and executed can serve in the "on demand" estimation of model right-hand-sides, of the action of "coarse slow" Jacobians as well as derivatives with respect to parameters, in the computation of coarse fixed points and their leading eigenvalues – in short, of exactly the quantities that a linear or nonlinear controller design algorithm would need evaluated through a macroscopic model (had such a model been available) to perform its task.

For our problem, we use the coarse timestepper in a coarse fixed point algorithm to converge on the desired coarse nominal equilibrium x_0; we then proceed as follows (remarkably, the algorithm is the same for the case of legacy dynamic simulators and coarse timesteppers of microscopic/stochastic models):

- Discretize the domain $D^n \subseteq R^n$ of the state-space, where a numerical solution of the feedback linearization problem is sought in a mesh of, say, N points.

- Write the transformation vector $S(x)$ as a power series expansion up to order p around the equilibrium x_0 i.e. write $S(x)$ as $S(x; h)$, where $h \in R^m$ is the vector of the power series coefficients. For example for a 2-dimensional problem $S(x; h) \equiv S(x_1, x_2; h)$ can be written as:

$$S_1(x_1, x_2; a_{i=1,\ldots p}) = a_1 x_1 + a_2 x_2 + \frac{1}{2!} a_3 x_1^2 + \frac{1}{2!} a_4 x_2^2 + a_5 x_1 x_2 + \ldots + O(p+1) \quad (28)$$

$$S_2(x_1, x_2; b_{i=1,\ldots p}) = b_1 x_1 + b_2 x_2 + \frac{1}{2!} b_3 x_1^2 + \frac{1}{2!} b_4 x_2^2 + b_5 x_1 x_2 + \ldots + O(p+1) \quad (29)$$

  where:

$$h = [a_1, a_2, \ldots, a_p, b_1, b_2, \ldots, b_p] \quad (30)$$

  Then, write the feedback control law as in (17).

- Calculate the values of the unknown coefficients of $S(x; h)$ using a matrix-free iterative nonlinear solver [Kelley, 1999], or possibly an unconstrained optimization algorithm, such as the Broyden, Fletcher, Goldfarb, Shanno (BFGS) method.

The optimization problem can be stated as finding the values of the vector h such that the sum of squared errors on the discretization mesh is minimized, i.e.:

$$\min_{h} \frac{1}{2} \sum_{i=1}^{N} \| G_i(h) \|_2^2 \tag{31}$$

where the vector function $G_i(h)$ is defined as: $G_i(h) = S(\Phi_T(x_i, -cS(x_i); h) - AS(x_i; h)$, $\forall x_i$ on the discretized mesh, and $\| \bullet \|_2$ is the standard Euclidean norm in the above minimum norm problem [Luenberger, 1969].

The quantities involved in the optimization computations (e.g. the values G_i) are evaluated repeatedly using the (legacy or coarse) timestepper for each value x_i in the mesh.

Remark 6: The single-step feedback linearization problem under consideration admits an alternative formulation, where the inverse transformation map: $x = w(z)$ is sought that satisfies the following system of NFEs:

$$\begin{aligned} w(Az) &= \Phi(w(z), -cz) \\ w(0) &= 0 \end{aligned} \tag{32}$$

where:

$$x = w(z) = S^{-1}(z) \tag{33}$$

The above functional equation is structurally simpler (first-order) than (12) (second-order), since in the latter the unknown vector function $S(x)$ appears through two consecutive function composition operations. Furthermore, it can be easily shown that the above problem reformulation leads to the same results, namely the same feedback linearizing control law [Kazantzis, 2001]. Notice, that in this case we expand $w(z)$ (instead of $S(x)$) in a power series and we then seek the values of the vector $h^{'}$ such that the sum of squared errors on the discretized domain (w.r.t z state-space, say $D^{'n} \subseteq R^n$) is minimized, i.e.:

$$\min_{h^{'}} \frac{1}{2} \sum_{i=1}^{N} \| G_i^{'}(h^{'}) \|_2^2 \tag{34}$$

where the vector function $G_i^{'}(h^{'})$ is defined as: $G_i^{'}(h^{'}) = w(Az_i) - \Phi_T(w(Az_i), -cz_i); h^{'})$, $\forall z_i$ on the discretized mesh.

Upon convergence we find the desired transformation $S(x)$ symbolically by applying a functional inverse on $w(z)$. More generally, matrix-free iterative linear algebra approaches can be used to solve the discretized nonlinear functional equations; in these methods the action of the Jacobian is estimated by appropriately initialized nearby initial conditions (dictated, for example, by a GMRES protocol). It is worth noting that, if the problem dynamics are characterized by a separation of time scales, and the long-term dynamics lie on

a low dimensional, attracting manifold, the dynamical integration involved in timestepping may be beneficial to the convergence of such iterative solution techniques [Wington et al., 1985; Kelley et al., 2004].

5 An Illustrative Case Study

5.1 The Deterministic Version

Our illustrative example consists of a simplified mechanism for the dynamics of NO reduction by H_2 on Pt and Rh surfaces. The simplified deterministic mean field model for this mechanism is given by:

$$\frac{dx}{dt} = \alpha(1-x) - \gamma x - u(1-x)^2 x \equiv L(x,u) \tag{35}$$

where x is the coverage of adsorbed NO, α is the rate constant for NO adsorption (incorporating the gas phase NO partial pressure), γ is the rate constant for NO desorption, and u is the reaction rate constant (and, in our scheme, the control variable). In order to transform the problem back to the discrete time formulation, we take a forward Euler step of the continuous time problem

$$x(k+1) = x(k) + TL(x(k), u(k)) \equiv \Phi(x(k), u(k)). \tag{36}$$

Simulation results were obtained for: $\alpha = 1, \gamma = 0.01$. This model, exhibits two regular turning points (at $u \simeq 3.96$ and $u \simeq 26$) as shown in the bifurcation diagram (Figure 2). We want to derive a nonlinear feedback control based on the proposed methodology, to stabilize the timestepper at the open-loop unstable stationary state ($x_0 = 0.5559, u_0 = 4$). We chose $T = 0.1$ as the reporting time horizon; the open loop eigenvalue at the nominal steady state is 0.1459, and the characteristic time is 6.85; A time step of 0.1 is therefore sufficient for accuracy of the Euler integration step and numerical stability.

5.2 The Microscopic/Stochastic Version

The procedure remains essentially the same when the timestepper results are obtained through short bursts of microscopic simulation. Here for the stochastic simulations of the mechanism embodied in (36) we used the Gillespie Stochastic Simulation Algorithm (SSA) [Gillespie, 1976, 1977].

Given the value of the surface coverage at time $t = 0$ we computed the expected value of the coverage after a reporting time horizon T by simulating a system with a relatively large number of available sites (say N_{size}), averaging over several realizations (say N_{run}); the

system size and number of realizations were chosen here to be $N_{size} = 100^2$ and $N_{run} = 100$, respectively. The time horizon was again selected to be $T = 0.1$. The Monte Carlo model is considered as a "black box" coarse timestepper $x(k+1) = \Phi_T(x(k), u(k))$.

The coarse Jacobian (here, a single derivative, which doubles as the coarse eigenvalue) at the fixed point is estimated by wrapping a Newton's method around the coarse KMC timestepper. The coarse identified model (Jacobian and right hand-side) is then used for tracing the solution branch by coupling to a pseudo-arc-length continuation scheme [Keller, 1977]. For the continuation we used $N_{size} = 200^2$ and $N_{run} = 1000$. For details on the computation of coarse stationary states and coarse bifurcation diagrams in an equation-free framework see [Makeev et al., 2002; Gear et al., 2002; Kevrekidis et al. 2003]. The resulting bifurcation diagram coincides with the one obtained through the deterministic timestepper. Given the unstable coarse stationary state at $u = 4$, the requisite functional equation for simultaneous feedback linearization and pole placement was solved using the coarse timestepper and minimizing Equation (30) using the BFGS method. To implement this procedure we used deviation variables defined as $x' = x - x_0$ and $u' = u - u_0$, while A now is a scalar chosen as 0.8.

We derived the unknown transformation map $S(x)$ numerically by the following distinct ways:

a) Analytically, by expanding $S(x)$ in a power series and retaining quadratic terms of the form $S(x) = \alpha_1 x + 0.5\alpha_2 x^2$, substituting $u = -S(x)$ into $\Phi(x(k), u(k))$ and then expanding $\Phi(x(k), -S(x))$ in Taylor series around the equilibrium (0,0). The values of the unknown coefficients α_i's are computed by equating terms of the same order on both sides of NFEs (12).

b) Equation-free by using the "black-box" KMC timestepper approach, i.e. by solving the optimization problem as appearing in (31) using the BFGS quasi-Newton method and a line search technique.

Here the domain of interest was chosen as $D \in R \equiv [-0.1 \;\; 0.1]$ and was discretized into 25 equally spaced points. In Figure 3 we plot the derived $S(x)$.

The transformation found by solving the NFE using timestepping is later used to close the loop (simultaneously linearizing and assigning poles for the closed loop system dynamics) Figure 4 demonstrates responses resulting from the desired closed loop dynamics $z(k+1) = S(k+1) = 0.8z(k) = 0.8S(k)$ (dotted lines) and that of the numerically obtained transformation $S(x)$ when applying the control law on the coarse KMC timestepper (solid ones). Figure 5 shows the *closed loop* responses of the deterministic mean field model and of the Kinetic Monte Carlo version starting from different initial conditions.

These were obtained through the solution of the norm minimization problem (31) using the deterministic and the stochastic KMC model respectively. The feedback linearizing transformation was found by minimizing (31) using the BFGS method. The obtained results confirm the effectiveness of the proposed equation-free nonlinear controller design methodology, demonstrating successful stabilization and regulation of the process at the unstable stationary state.

6 Concluding Remarks

We demonstrated how feedback linearization with pole placement in a single step, analyzed in [Kazantzis, 2001] for closed form equation models, can be performed in an equation-free framework by acting directly on a fine scale simulator. The illustrative example used a stochastic realization of a simplified model of a catalytic surface reaction. Admittedly, the example is a very simple one; in particular, it is (coarsely) one-dimensional, and for such systems a feedback linearization transformation always exists [Isidori, 1999]. Yet the timestepper based, equation-free methodology illustrated is not restricted to one dimensional (when coarse-grained) problems; all the elements of the method (the timestepper, the location of unstable fixed points and their leading slow eigenvalues, the solution of the corresponding functional equation) remain effectively the same in higher-dimensional cases. More sophisticated matrix-free iterative methods can be used to solve the requisite functional equation by acting directly on the fine-scale simulator. Parallel computation (a different replica fine scale simulation of the same initial condition performed on each processor) and computational tools like *In situ Adaptive Tabulation* (ISAT, [Pope, 1997]) can be used to alleviate, when appropriate, the computational wall clock time and effort required to estimate the necessary coarse-grained quantities. Furthermore, if a strong separation of time scales (a spectral gap) appears in the coarse-grained dynamics, and the long-term behavior lies on a low-dimensional "slow manifold", it is possible to take advantage of this through timestepping to solve an effective NFE of reduced dimension [Gear et al., 2004]. In this paper we assumed that we knew what "the right" macroscopic observable was, in which to restrict the microscopic system dynamics; the detection of appropriate such observables, either through data analysis [Coifman et al., 2004] or observer design is a subject we are currently pursuing.

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Figure Captions

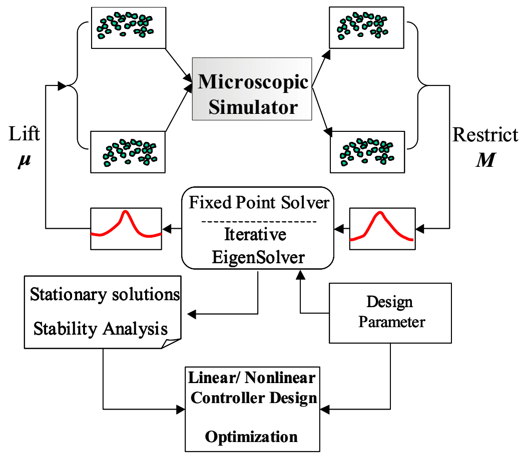
Figure 1: Schematic of the coarse timestepper in a controller design framework

Figure 2: (a) Coarse Bifurcation diagram of the kMC model, obtained by the coarse timestepper, (b) blow up of the diagram near the equilibrium of interest; solid lines correspond to stable coarse steady states while the dotted ones correspond to unstable coarse steady states

Figure 3: $S(x)$ as computed analytically (solid line) and using the black-box coarse KMC timestepper (dotted line)

Figure 4: Transients of $S(k+1) = 0.8S(k)$, corresponding to the desired closed loop dynamics, (solid lines) and $S(x(k))$ using the computed control law on the coarse KMC timestepper (dotted lines)

Figure 5: (a) Transient response for 0.1 initial perturbation of the coarse state variable from the coarse equilibrium. (b) Transient response for 0.2 initial perturbation of the coarse state variable from the coarse equilibrium, (c) Transient response of the control variable for 0.2 initial perturbation of the coarse state variable from the coarse equilibrium (lower ones correspond to -0.2). Simulation runs for the KMC timestepper were obtained with $N_{size} = 100^2$ and $N_{run} = 100$.


Microscopic Simulator
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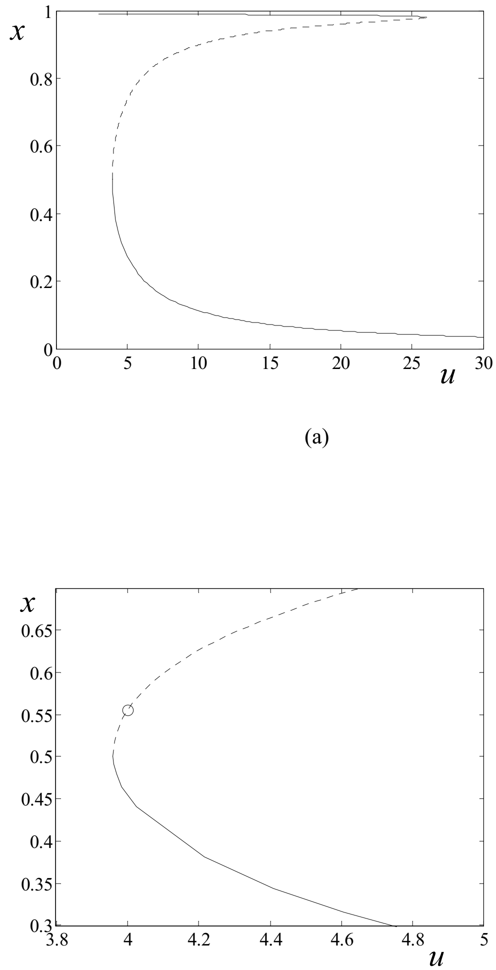
Fixed Point Solver
Iterative EigenSolver
Stationary solutions
Stability Analysis
Design Parameter
Linear/ Nonlinear Controller Design
Optimization



(a)

(b)

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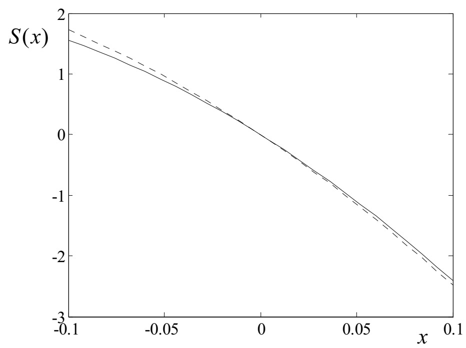
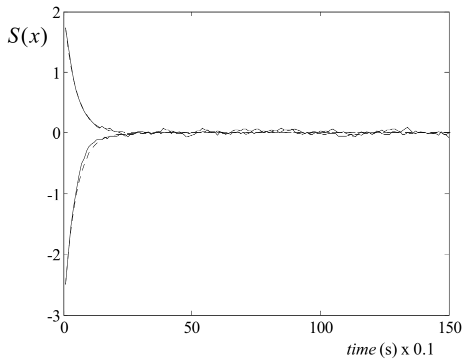


Figure 3: $S(x)$ as computed analytically (solid line) and using the black-box coarse KMC timestepper (dotted line).



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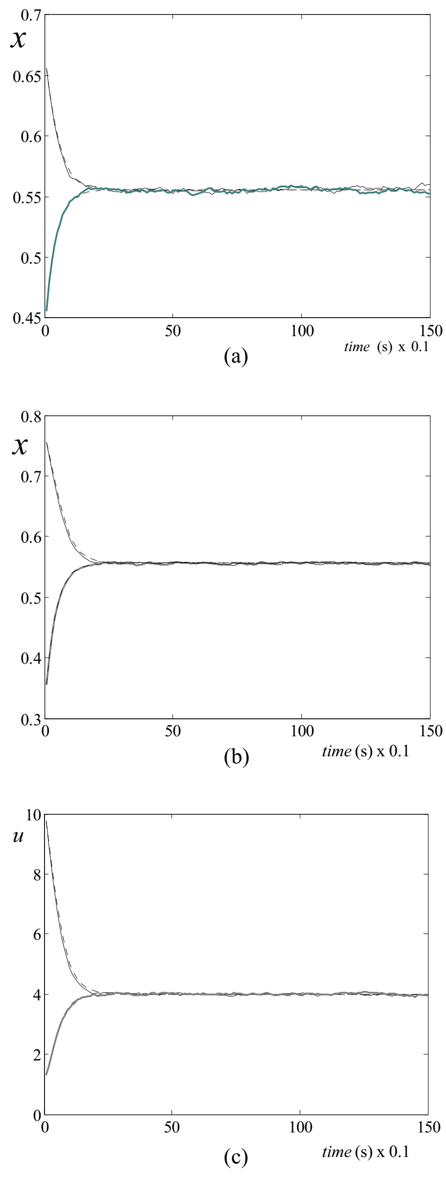

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